The spin-1/2 anisotropic Heisenberg-chain in longitudinal and transversal magnetic fields: a DMRG study.

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Abstract. Using the density matrix renormalization group technique, we evaluate the low-energy spectrum (ground state and first excited states) of the anisotropic antiferromagnetic spin-one-half chain under magnetic fields. We study both homogeneous longitudinal and transversal fields as well as the influence of a transversal staggered field on opening of a spin-gap. We find that only a staggered transversal field opens a substantial gap.

1 Introduction

Recently, the properties of low-dimensional quantum spin systems in longitudinal, transversal and/or staggered magnetic fields have become of considerable interest. To give an example, the two-dimensional compound $SrCu_2(BO_3)_2$ is a realization of the Shastry-Sutherland model [1], close to quantum-criticality, with a spin gap of 31 K which shows magnetization plateaus in an external field [2].

Most spin-1/2 systems show little anisotropies in the magnetic exchange. The discovery [3] that low-dimensional magnetic excitations in the rare-earth compound Yb_4As_3 can explain the large linear specific heat coefficient γ in this low-carrier half-metal [4,5] opens the possibility to study in deeper detail the properties of a rare-earth quantum-spin-chain-system with its enhanced magnetic anisotropies [6,7].

Inelastic neutron scattering experiments [8] on Yb_4As_3 found a gap to (all) magnetic excitations opening in the presence of an external magnetic field, confirming a prediction [3] by Schmidt *et al* based on an interpretation of previous specific heat data [9]. Several proposals have been made in order to explain this very unusual behavior [10]. The first model [3] is based on inter-chain interactions. The second model [11] is based on the observation that a staggered Dzyaloshinsky-Moriya (DM) interaction, which generates an effective staggered g-tensor, is allowed [6,7] in the $4f$-compound Yb_4As_3. It is know that a staggered g-tensor leads to a gap in an external field [12,13]. The third model [10], based on a mean-field analyze of the anisotropic spin-chain, proposes that a gap opens in the presence of a uniform transversal magnetic field.

Here we will analysis the two latter proposals by a systematic DMRG-studies of the relevant models. We find that only the effective staggered g-factor-model is able to explain the field-dependent opening of a spin-gap in Yb_4As_3.

1.1 Model and method

The magnetic properties of Yb_4As_3, in the absence of an external magnetic field, are well described by an antiferromagnetic Heisenberg spin-1/2 chain. Switching on the external magnetic field, experimental data shows the opening of a gap in the low energy excitation spectrum. However, the standard Heisenberg model in an applied field remains gapless from zero magnetic field up to the saturation magnetization. The anisotropic Heisenberg model

$$H = \sum_{i=1}^{L-1} J_{xy} \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right) + J_z S_i^z S_{i+1}^z$$
$$- \sum_{i=1}^{L} h_x S_i^x + \sum_{i=1}^{L} h_x^{stag} (-1)^i S_i^x - \sum_{i=1}^{L} h_z S_i^z \qquad (1)$$

with an uniform transversal field h_x, a staggered transversal field h_x^{stag} and a longitudinal field h_z incorporates all features proposed [10,11] to be relevant for Yb_4As_3. The magnetic fields appearing in (1) include the gyromagnetic g-factors.

The staggered transversal field in (1) is induced by a staggered Dzyaloshinsky-Moriya interaction given by the term $\sum_i (-1)^i \mathbf{D} \cdot (\mathbf{S}_i \times \mathbf{S}_{i+1})$. Setting $D = |\mathbf{D}| = J_z \sin(2\theta)$ the DM-term can be eliminated [12,14] by a rotation around $\mathbf{D}$ by an angle θ leading to $h_x^{stag} = \sin(\theta) h_z$, which can be interpreted as an effective staggered g-tensor.

We have simulated the anisotropic Heisenberg model (1) using the Density Matrix Renormalization Group (DMRG) technique [15]. We have, in general, investigated carefully the dependence of the results on the number m of states kept in the DMRG calculations. If not stated otherwise, we have used open boundary conditions, the finite-system-size algorithm and extrapolated the finite-size data to the thermodynamic limit, setting $J_{xy} \equiv 1$ in (1).
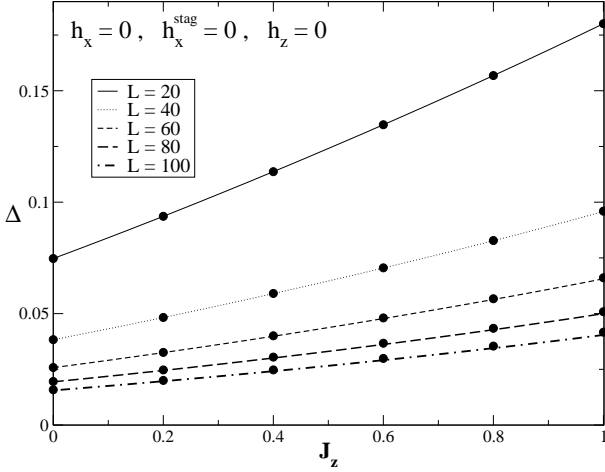
Fig. 1. Comparison between DMRG results (filled circles) for the finite-size gap $\Delta(L)$, using $m = 50$ states, and the Bethe-Ansatz results (lines). The gap is given as a function of the anisotropy J_z in the absence of external magnetic fields.

1.2 Comparison of DMRG and Bethe-Ansatz results

In order to verify the accuracy of our approach for the excitation energies we use the Bethe-Ansatz equations [18, 19] to evaluate the gap $\Delta(L)$ for finite chains with size L,

$$\Delta(L) = E_1(L) - E_0(L) \ ,$$

for the anisotropic antiferromagnetic Heisenberg chain and then compare it with our DMRG simulations. In Fig. 1 we plot the finite-size gap obtained by using DMRG versus the anisotropy ($0 \leq J_z \leq 1$), the lines correspond to the exact finite-size gap obtained using Bethe-Ansatz. Although in this regime the gap in the thermodynamic limit is equal to zero, the correspondence between our DMRG simulations for the gap for finite system sizes with the Bethe-Ansatz results is very accurate.

2 Homogeneous transversal magnetic field

Uimin *et al* proposed, by a mean-field calculation [10], that a gap opens for the spin-1/2 anisotropic Heisenberg chain

$$H = \sum_{i=1}^{L-1} J_{xy}(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + J_z S_i^z S_{i+1}^z$$

$$-h_x \sum_{i=1}^{L} S_i^x \qquad (2)$$

in the presence of a homogeneous longitudinal field h_x. This mean-field result would then imply that no further magnetic anisotropies would be needed to explain the experimentally observed spin-gap of Yb_4As_3.

In spin-wave theory Uimin *et al* found [10] for the model (2) a gap Δ_{SWT} consisting of two branches:

$$\Delta_{SWT} = \min(\Delta_1, \Delta_2) \ ,$$

with $\Delta_1 = h_x$ and

$$\Delta_2 = \sqrt{\frac{2}{3}\left(\frac{1-J_z}{2+Jz}\right)\left((2+J_z)^2 - \left(\frac{3h_x}{2}\right)^2\right)} \ . \qquad (3)$$

Up to a certain magnetic field the value of the gap is almost linear and above this value the gap starts to close itself following a quadratic form, compare Fig. 4 and Fig. 5.

The physical reasoning for the gap present in the mean-field results reviewed above is the following: neglecting the $S_i^x S_{i+1}^x$ coupling term in the Hamiltonian (2) it becomes identical to the Ising model in a transversal field, which has a two-fold degenerate ground-state and a gap. It has been argued [16,17], that this reasoning remains valid also for (2).

We compute the energy gap $\Delta(L)$ using the DMRG. We calculate the ground state and the lowest excited states energies $E_i \, (i = 0, 1, 2)$ and form the following energy difference $\Delta_1 = E_1 - E_0$ and $\Delta_2 = E_2 - E_0$ respectively between the first and the second excited state with the ground state energy. Fig. 2 and Fig. 3 show the behavior of $\Delta_i(L)$ with the transverse magnetic field h_x for $J_z = 0.75, \ 0.9706$.

In the thermodynamic limit the first energy difference $\Delta_1 \to 0$ in the low magnetic field regime ($h_x \ll 2$). This behavior is in agreement with the fact that the GS is doubly degenerated in this regime when $L \to \infty$. Thus to estimate the eventually system-gap in this regime we calculate Δ_2. Δ_2 shows a more monotonous behavior. For fixed h_x, $\Delta_2(L)$ is decreasing with the system-size L ($\Delta_2(100) \leq 0.04$). Fig. 4 and Fig. 5 show the extrapolate gap for the thermodynamic limit with $J_{xy} = 1$ and $J_z = 0.75, 0.9706$. We have evaluated also the induced uniform magnetization M_x, which we present in Fig. 6 for $J_z = 0.25$ and $J_z = 0.9706$ (value which corresponds to the small anisotropies in xy-plane appropriate for Yb_4As_3 [3]).
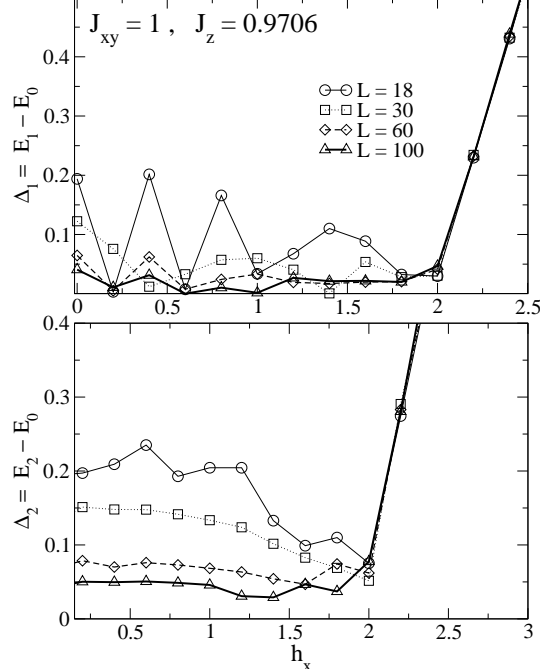
We observe:

i) The DMRG data presented in Fig. 4 and Fig. 5 (open circles) show a phase diagram divided in two regions well separated by a critical magnetic field, which depends on J_z and which is around $h_x \simeq 2$ for $J_z \simeq 1$ in agreement with the isotropic case [20].
    For h_x below the critical magnetic field the system appears gapless. For h_x above the critical magnetic field, a linear gap opens corresponding to the classical ferromagnetic phase, polarized along x-direction.

ii) As it appears in the Fig. 4 and Fig. 5, where we plot the spin-wave theory gap (open diamonds), there is a substantial disagreement between our DMRG-simulation and SWT prediction [10].

iii) We find that the induced magnetization M_x saturate for h_x larger than the critical field, as illustrated in Fig. 6 for $J_z = 0.25$ and $J_z = 0.9706$ (and the staggered magnetization reduces to zero [21]). This explains the opening of a gap linear in h_x in this phase.
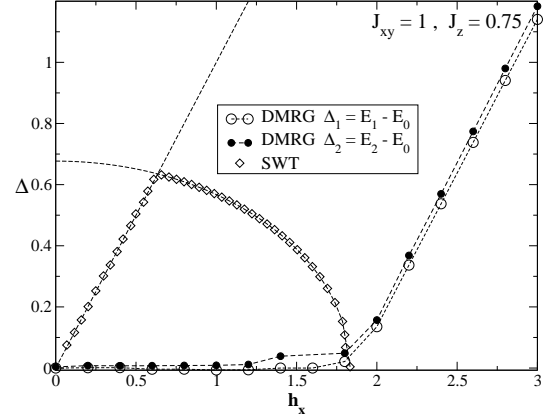
Dmitriev *et al* have used scaling arguments [17] and found for the Hamiltonian (2) that a gap $\Delta \sim (h_x)^\nu$
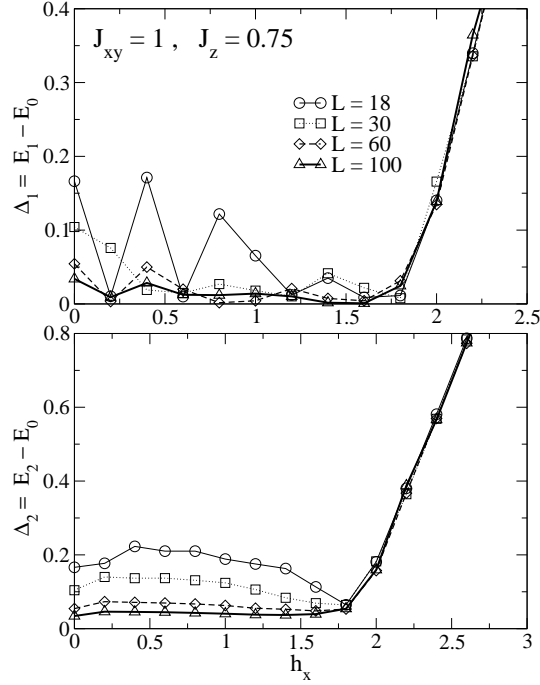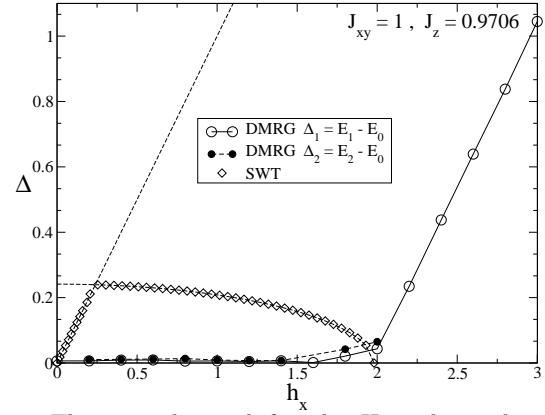
Fig. 2. Finite-size gaps observed for the Heisenberg chain of size L in a transversal magnetic field h_x with $J_{xy} = 1$, $J_z = 0.75$.


Fig. 3. Finite-size gaps observed for the Heisenberg chain of size L in a transversal magnetic field h_x with $J_{xy} = 1$, $J_z = 0.9706$.

Fig. 4. The gap observed for the Heisenberg chain in a transversal magnetic field h_x with $J_{xy} = 1$, $J_z = 0.75$. The circle symbols come from DMRG simulations ($m = 50$) extrapolated to the thermodynamic limit. The diamond symbols represent induced gap calculated from spin-wave theory.

Fig. 5. The gap observed for the Heisenberg chain in a transversal magnetic field h_x with $J_{xy} = 1$, $J_z = 0.9706$. The circle symbols come from DMRG simulations ($m = 50$) extrapolated to the thermodynamic limit. The diamonds represent the induced gap calculated from spin-wave theory.
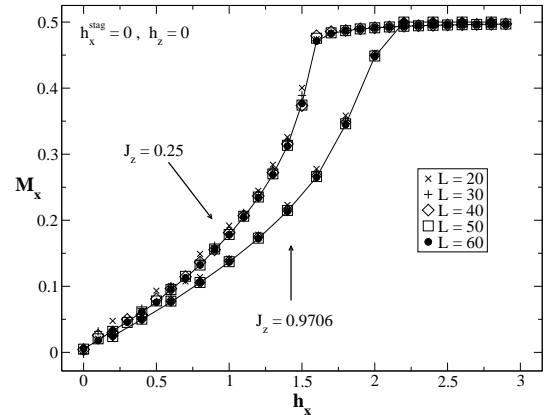
Fig. 6. The magnetization M_x along x for a anisotropy $J_z = 0.25$, 0.9706. Note the saturation of M_x above a certain critical field.

opens for small external magnetic field, with an exponent ν depending on the anisotropy. Our simulations for small anisotropy are not supporting these predictions [17,22]. But due to the difficulty to resolve accurately Δ_2 using DMRG, we cannot exclude completely an eventual small gap. Although till now we are not able to give a clear answer to the gap-opening question, but at least it seems that if there is a gap, the prefactor of the scaling law would need to be very small and in any case too small to explain experimental results on Yb_4As_3.

3 Staggered magnetic field

3.1 Model

The staggered Dzyaloshinsky-Moriya interaction, which is allowed [6,7,11] in the $4f$-compound Yb_4As_3, leads in an external homogeneous magnetic field h_z to an effective transversal staggered field h_x^{stag}. In this context the anisotropy is not relevant and we can consider the (isotropic) Heisenberg case $J_{xy} = J_x \equiv J$:

$$H = J \sum_{i=1}^{L-1} \mathbf{S_i} \cdot \mathbf{S_{i+1}} + h_x^{stag} \sum_{i=1}^{L} (-1)^i S_i^x - h_z \sum_{i=1}^{L} S_i^z . \quad (4)$$

The above Hamiltonian is not invariant under reflection with respect to the mid point of the chain when L is even. However in the standard implementation of the DMRG algorithm, L is even and the reflection symmetry is used. The Hamiltonian (4) can be easily made invariant under reflection by means of a local rotation, given by:

$$\begin{pmatrix} (-1)^i S_i^x \\ (-1)^i S_i^y \\ S_i^z \end{pmatrix} \rightarrow \begin{pmatrix} S_i^x \\ S_i^y \\ S_i^z \end{pmatrix} .$$

The transformed Hamiltonian reads:

$$H = J \sum_{i=1}^{L-1} \left[S_i^z S_{i+1}^z - \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right) \right]$$
$$+ h_x^{stag} \sum_{i=1}^{L} S_i^x - h_z \sum_{i=1}^{L} S_i^z \quad (5)$$

3.2 Effect of the staggered transversal field

We start by analyzing the finite-size dependence of the energy gap. The Fig. 7 shows the behavior of the finite size system gap versus the staggered magnetic field. One can clearly observe (i) that the gap vanishes in the thermodynamic limit only for zero h_x^{stag} and (ii) that the magnetic correlation length is large but finite in the gapped case $h_x^{stag} > 0$; the data for larger system size L is essentially flat for $h_x^{stag} > 0$.

In Fig. 8 we show the magnetization along the z-direction as a function of h_z, for various h_x^{stag}. Since $J_{xy} =$
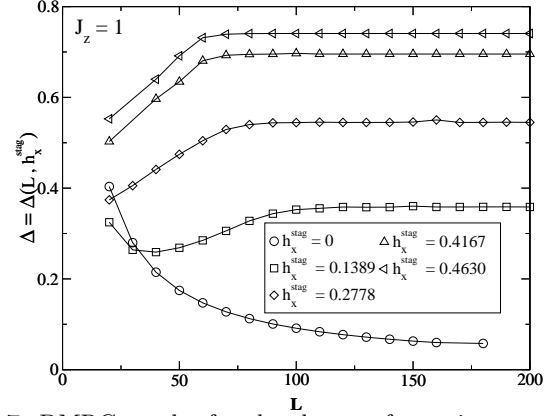

Fig. 7. DMRG results for the the gap for various staggered fields h_x^{stag}, as a function of chain length L, for $h_z = 0$.
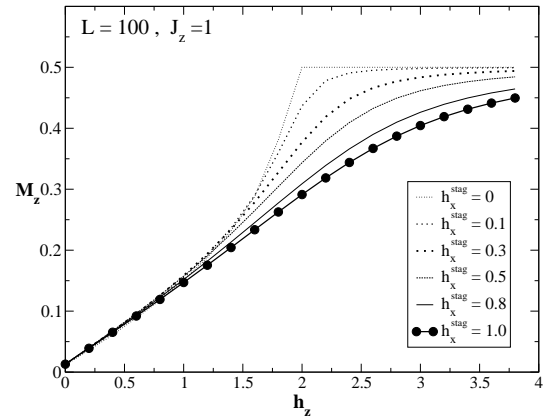

Fig. 8. Magnetization curves along the z-direction, compare [14].

$J_x \equiv 1$ in (5), these results can be compared directly to those given in Fig. 6 for fields along x-direction. We note that the second-order phase transition to a completely magnetized state occurring at $h_z = 2$ in the absence of a staggered field is progressively smeared out by h_x^{stag}; the transversal field induces quantum fluctuations into the magnetized state. These results confirm a similar study [14]

3.3 Comparison with experiment

Now using the experimental estimation for exchange coupling in the isotropic Heisenberg chain $J \simeq 26\,K$, we fit the experimental data for the gap. The staggered magnetic field h_x^{stag} is proportional to the experimental magnetic field H^{ext} via $h_x^{stag} = c_0 \sin(\theta) H^{ext} = c_0/g_\perp \sin(\theta) h_z$, where $g_\perp$ is g-factor for a magnetic-field perpendicular to the chain-direction. The g-factors for Yb_4As_3 are very anisotropic, $g_\perp$ has been estimated to be [14] $g_\perp \approx 1.3$.

Our fit yields $c_0/g_\perp \sin(\theta) \simeq 0.18$. The fitting to experimental data depends on c_0 which has not yet been determined precisely by experiment. While in the literature [11] $c_0 \simeq 0.27$, we get a good agreement with our DMRG simulations and the experimental curve for $c_0 \simeq 0.23$ (assuming $g_\perp \simeq 1.3$)(Fig.9).
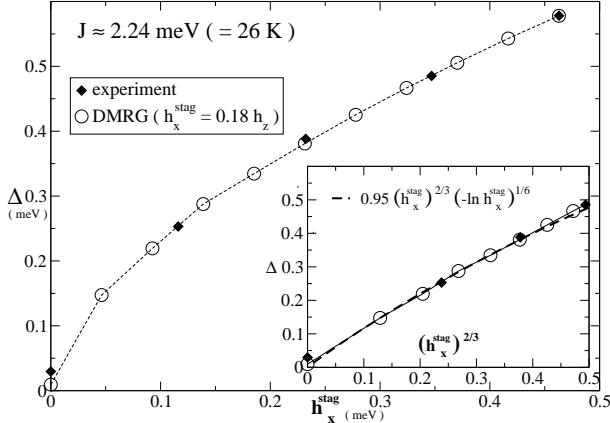
Fig. 9. Fit to experiment with data ($m = 70$) extrapolated to the thermodynamic limit.

3.4 General case

We consider now the case where the staggered and the uniform magnetic field are not proportional. We want to explore the excitation gap of

$$H = \sum_{i=1}^{L-1}(\mathbf{S_i} \cdot \mathbf{S_{i+1}} - \delta S_i^z S_{i+1}^z) + h_x^{stag}\sum_i^L (-1)^i S_i^x - h_z \sum_i^L S_i^z . \tag{6}$$

In Fig. 10 we present for $h_z = 0$ the gap Δ as a function of the anisotropy δ and the parameters a_0 and a_1 entering in the scaling-law

$$\Delta = a_0 \left(h_x^{stag}\right)^{a_1} \tag{7}$$

for the gap. Bosonization predicts [12,13] $a_0 \approx 1.85$ and $a_1 = 2/3$ for the isotropic case ($\delta = 0$, $h_z = 0$) for small staggered magnetic field h_x^{stag}. For the isotropic case ($\delta = 0$) we present in Fig. 11 the same data as a function of h_z.

We also examined the DMRG-data using (7) including multiplicative logarithmic corrections [12,13]: $\Delta = a_0 \left(h_x^{stag}\right)^{a_1} |\log h_x^{stag}|^{1/6}$ We found essentially the same values for the parameters a_0 and a_1 as presented in Fig. 10 and Fig. 11. We note, that (7) hold only in the asymptotic limit $h_x^{stag} \to 0$, which we do not examine in the present study. The results presented in Fig. 10 and Fig. 11 show a_0 and a_1 as obtained for overall fits to the gap, for $h_x^{stag} \leq 0.8$. We believe this parameter-region to be experimentally relevant.

4 Conclusions

We have studied the anisotropic Heisenberg-chain with staggered and uniform transversal and uniform longitudinal field by DMRG. We found no evidence for a substantial gap opening for a homogeneous transversal field, as predicted by a mean-field [10] and a scaling [17] analysis. We found, however, a gap opening for a staggered transversal field, in accordance with previous studies [12,13]. These results lead to the conclusion, that the gap-opening in
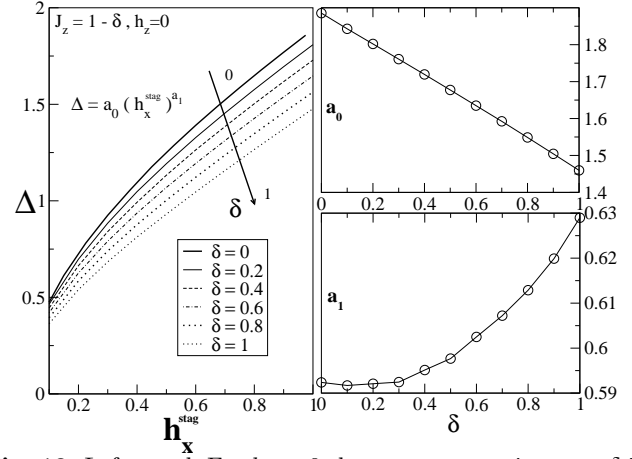
Fig. 10. Left panel: For $h_z = 0$ the gap versus anisotropy δ in the thermodynamic limit ($m = 40$). Right panels: Dependence of the parameters a_0 and a_1 as a function of δ.
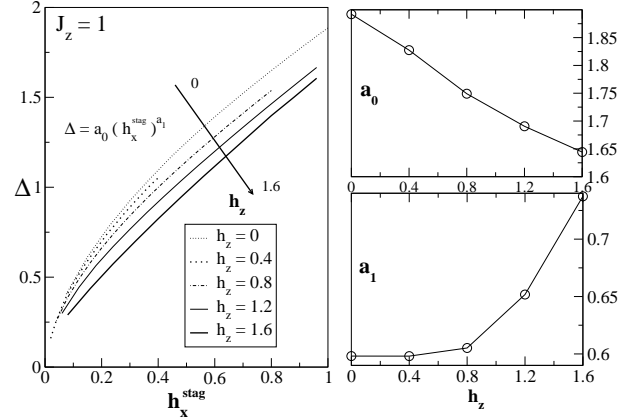
Fig. 11. Left panel: For $\delta = 0$ the gap versus uniform longitudinal field h_z in the thermodynamic limit ($m = 40$). Right panels: Dependence of the parameters a_0 and a_1 as a function of δ.

the the rare-earth, $4f$-compound Yb_4As_3 compound in an external magnetic field is attributable to a staggered Dzyaloshinsky-Moriya tensor [11,6,7].

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